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Title: Multigroup Scattering in Monte Carlo Radiation Transport Codes

Author(s): Singh, Luquant
Nelluvelil, Eappen Sebastian
Burke, Timothy Patrick
Trahan, Travis John

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Multigroup Scattering in Monte Carlo Radiation Transport Codes

Students: Eappen Nelluvelil and Luquant Singh
Mentors: Timothy Burke and Travis Trahan

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Final Presentations
August 10-12, 2021

Luquant Singh

- 2nd year electrical engineering PhD student at UW-Madison
  - Member of Helically Symmetric Experiment plasma lab studying turbulence in fusion plasmas
  - Broadly interested in HPC, fluid dynamics, astrophysics

- Undergraduate degree in applied math and physics, also at UW
  - clarinet performance

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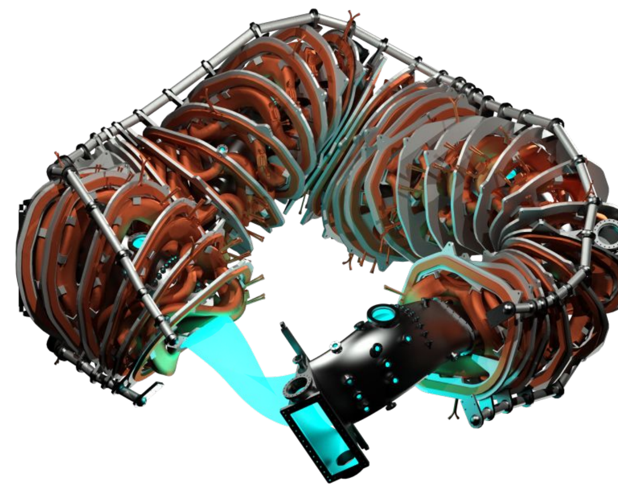
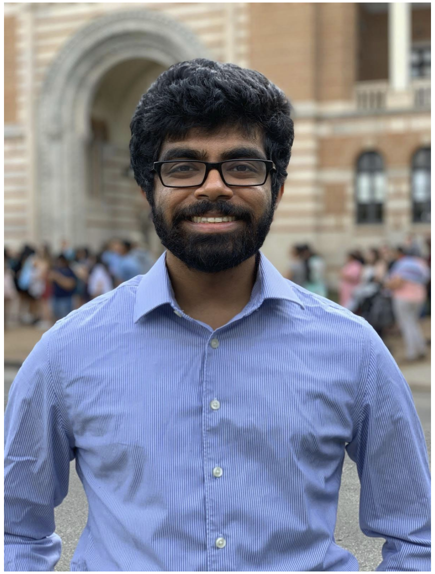


Eappen Nelluvelil

- Majored in computational and applied mathematics at Rice University
- Incoming 1st year applied mathematics PhD student at CU Boulder
  - Broadly interested in numerical linear algebra, numerical methods for PDEs, and high-performance computing



Evolution of a neutron population in the presence of material is governed by the neutron transport equation.

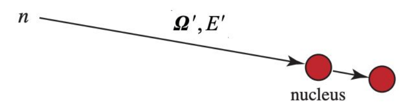
- When a neutron is incident on a material nucleus, three *neutron events* are most common:

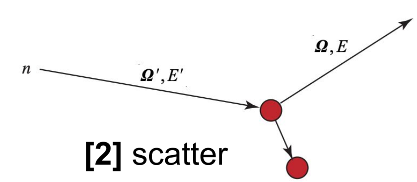
  [1] capture **[2]** scatter **[3]** fission

  – likelihood of an event proportional to corresponding *nuclear cross section*

- The *neutron transport equation* is a conservation law for neutron flux that depends on nuclear cross sections for capture, scattering, and fission

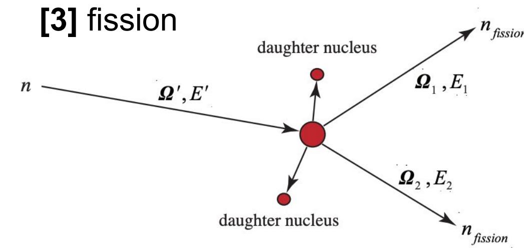
[1] capture





[2] scatter

[3] fission



Reproduced from Larsen, NERS 543 Lecture notes, Univ. of Michigan (2012)

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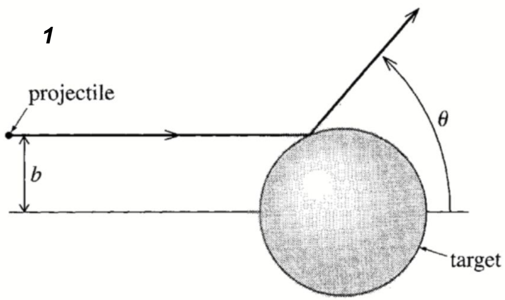
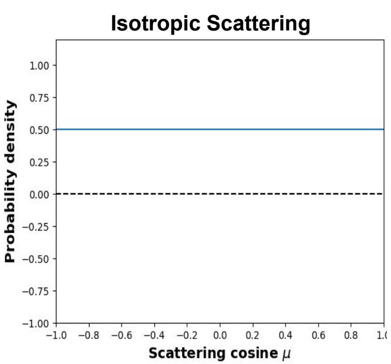
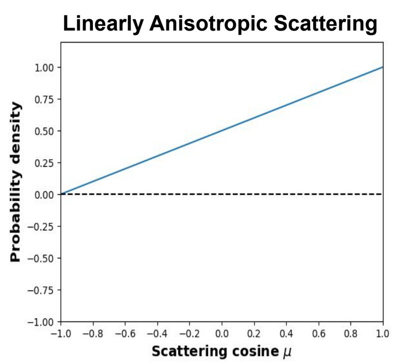
Neutron scattering is described by an angular probability distribution function.



$$\mu = \cos(\theta)$$
$$\theta \in [0, \pi]$$
$$\mu \in [-1, 1]$$





- In a scattering event, a neutron scatters an angle θ into an outgoing trajectory
- Every nuclear isotope has a unique scattering distribution derived from nuclear scattering cross section
  - represented in terms of *scattering cosine* μ
  - azimuthal symmetry → distribution functions depend only on scattering cosine

[1] *Reproduced from Fratus, PHYS 103 Lecture notes, Univ. of California (2015)*

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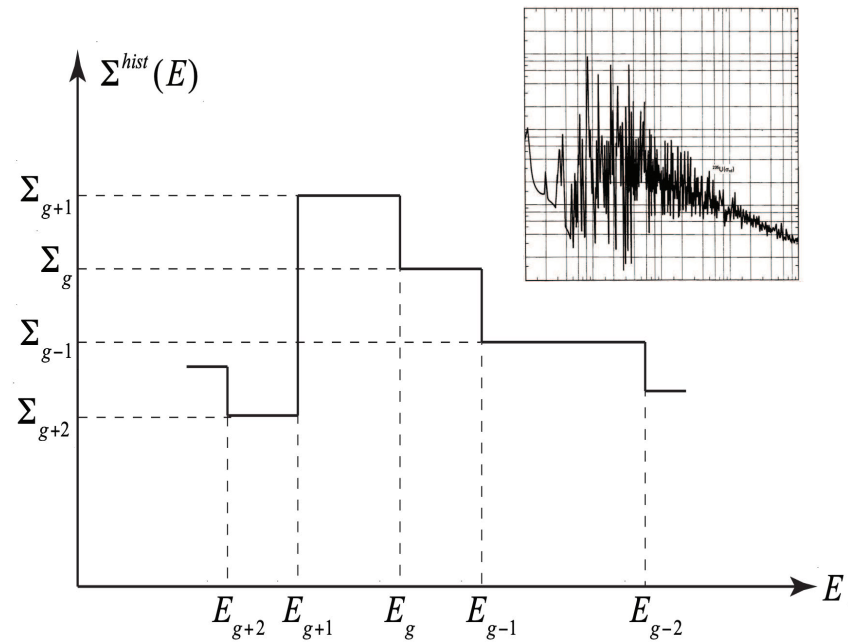
Several codes at LANL can determine approximate solutions to the neutron transport equation.

- Deterministic codes discretize in energy, angle, and time to obtain solutions
  - *multigroup approximation* is widely used for efficient calculations
  - each group-to-group transfer has a scattering distribution

- Monte Carlo codes determine transport quantities by sampling probability distributions
  - large number of neutrons are evolved using random numbers



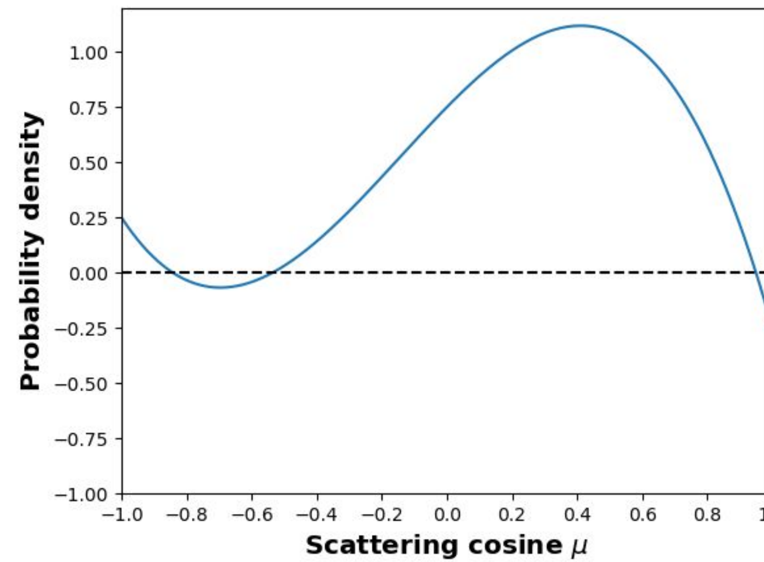
Adapted from Larsen, NERS 543 Lecture notes, Univ. of Michigan (2012)

Multigroup codes represent scattering distributions in terms of Legendre polynomials.

- Legendre polynomials are used to represent scattering PDFs because:
  - domain [-1,1] is same as scattering cosine range
  - efficient to only use low-order truncations of scattering distribution

- **Important:** low-order truncations of scattering distributions may be nonpositive over [-1,1]
  - not suitable for Monte Carlo sampling!

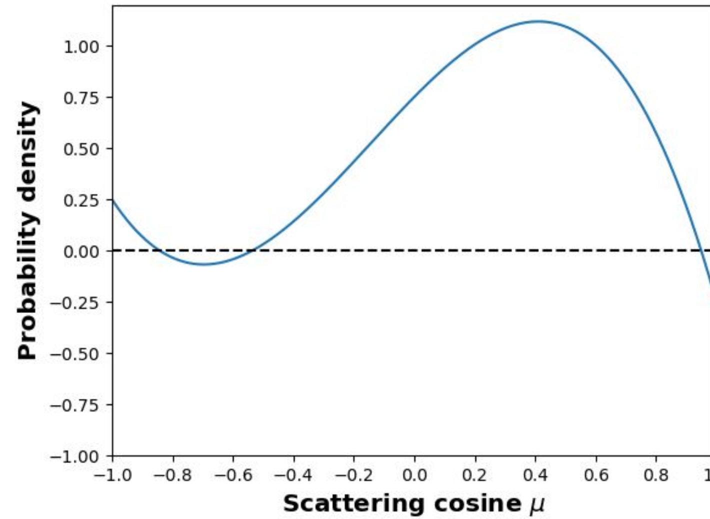
$$f_{g' \leftarrow g}(\mu) = \sum_{\ell=0}^{L} \frac{2\ell+1}{2} f_{\ell, g' \leftarrow g} P_\ell(\mu)$$



Moments of a scattering PDF describe angular anisotropy of scattering.

- We seek a non-negative PDF that captures the anisotropy of the truncated multigroup PDF
  - to capture PDF shape, we can compute moments of the distribution function
  - moments can be computed directly from Legendre coefficients

- Higher order moments capture higher order anisotropy



$$
\begin{aligned}
f_0 &= 1.0 & \qquad & \mathcal{M}_0 = 1.0 \\
f_1 &= 0.3 & \Rightarrow & \mathcal{M}_1 = 0.3 \\
f_2 &= -0.2 & & \mathcal{M}_2 = 0.2 \\
f_3 &= -0.2 & & \mathcal{M}_3 = 0.1
\end{aligned}
$$

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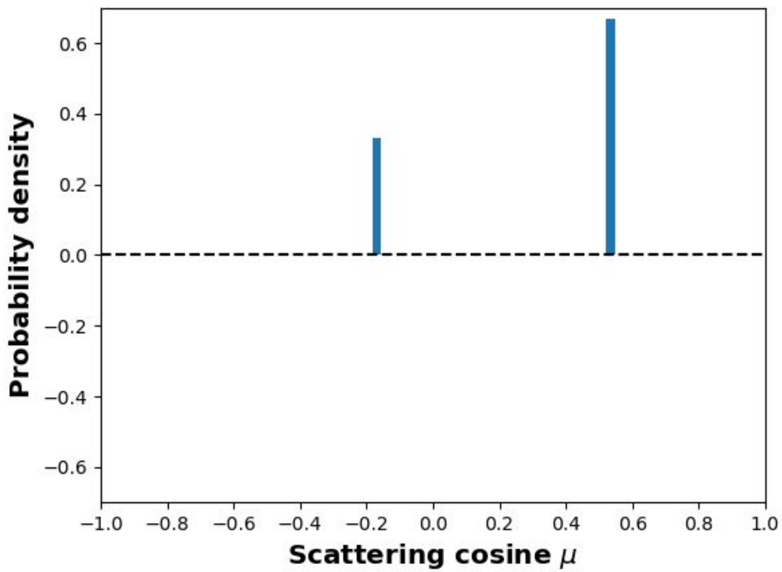
Using a discrete angle method, particles scatter into only a limited number of outgoing angles.

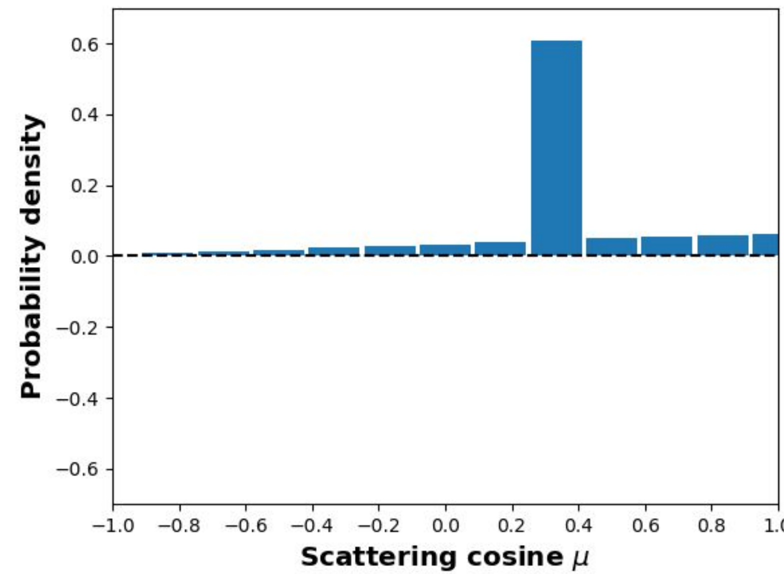


$$f(\mu) = \sum_{k=1}^{K} \omega_k \delta(\mu - \mu_k)$$

- Discrete angle technique (DAT) involves deriving a weighted delta function PDF
  - **Pros:**
    - fast sampling
    - for high-order truncations, anisotropy is well-represented
  - **Cons:**
    - low-order truncations may suffer from limited angle selection (ray effects)

For low-order truncations, a semicontinuous scattering distribution may best represent angular anisotropy.

- The semicontinuous (SC) method involves deriving a PDF that is a weighted sum of a continuous density and a delta function density
  - **Pros:**
    - weighting β of continuous and discrete densities can be specified
    - may mitigate low-order ray effects possible with DAT
  - **Cons:**
    - less efficient sampling
    - difficult to generalize



$$f\left(\mu\right) = \beta f^{*}\left(\mu\right) + \left(1-\beta\right)\left(\sum_{k=1}^{K} \tilde{\omega_k}\delta\left(\mu - \tilde{\mu_k}\right)\right)$$

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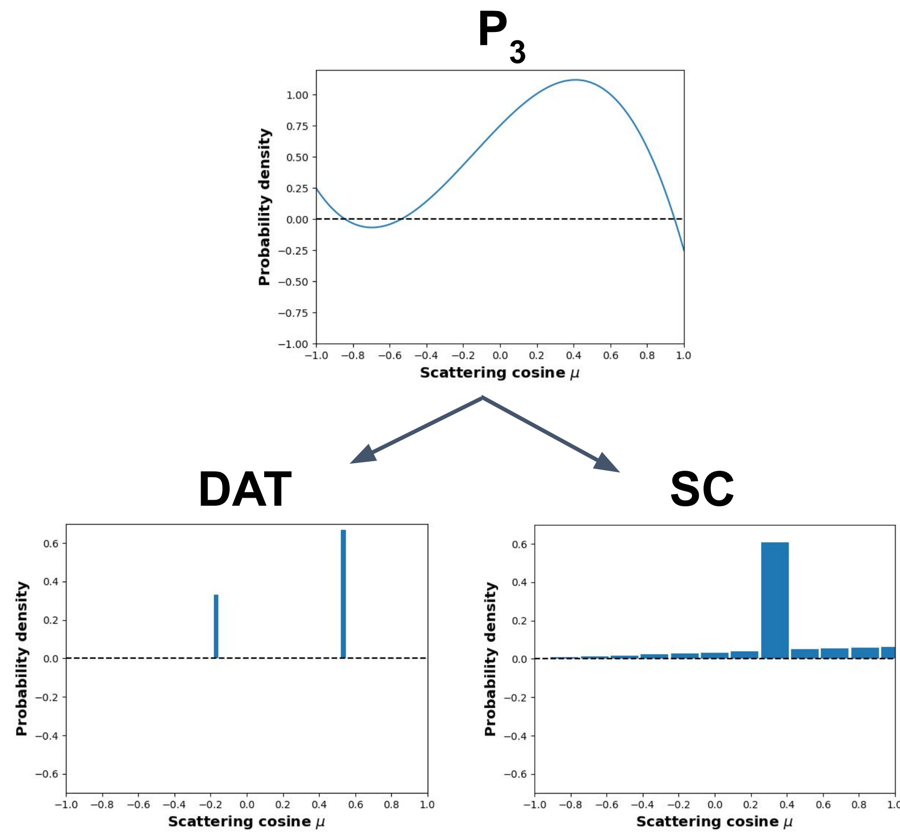
SC and DAT methods have been implemented in the GPU-enabled neutron transport code `MGMC`.

- Previously, **`MGMC`** used only isotropic P_0 sampling
  - only a good approximation in limited scenarios

- We implemented SC and DAT sampling for P_1 and P_3 PDFs
  - better captures anisotropic neutron scattering mechanics
  - can efficiently sample these PDFs on CPUs and GPUs



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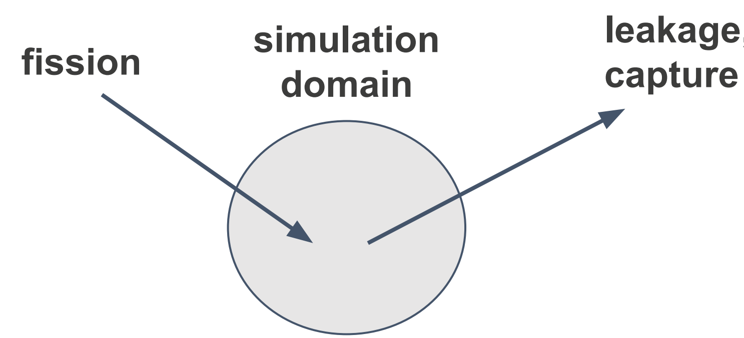
MGMC SC and DAT methods have been verified against other LANL codes using *k*-eigenvalue simulations.

- *k*-eigenvalue is a measure of criticality in a system
  - *k* = 1 critical
  - *k* < 1 subcritical
  - *k* > 1 supercritical

- To verify the SC and DAT methods in **MGMC**, *k* was computed for three critical ICSBEP benchmarks
  - results are compared with reference multigroup answers from deterministic code **PARTISN**



Benchmarks:
- IEU-MET-FAST-007 (BIGTEN)
- U233-SOL-THERM-008
- PU-MET-FAST-006 (FLATTOP)

Simulation parameters:
- 30 groups
- S_N = 128
- Particles/batch = 2^{20}, 400 batches

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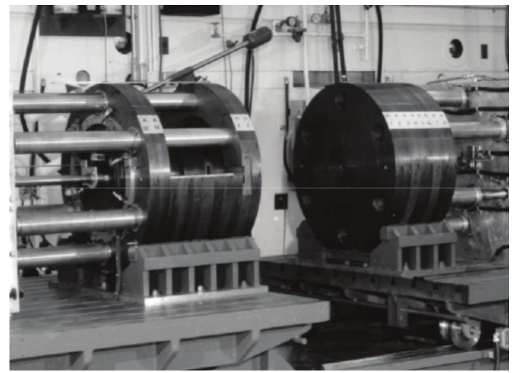
MGMC SC and DAT methods have been verified against other LANL codes using *k*-eigenvalue simulations.

PU-MET-FAST-006 (FLATTOP)

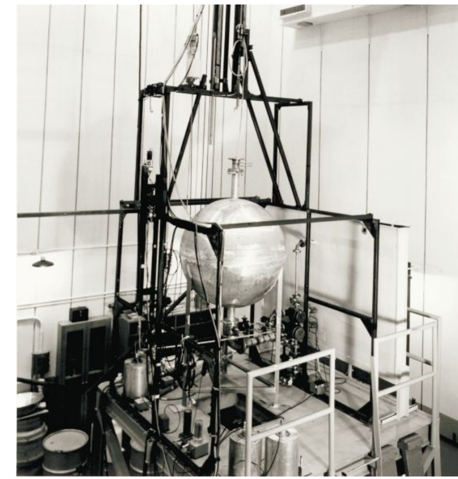
- 1.8in diameter ^{239}Pu metal alloy surrounded by 3.6in diameter Ni-coated U reflector

IEU-MET-FAST-007 (BIGTEN)



- **Big:** 10 metric tons of mixed Uranium, 6in thick depleted Uranium reflector; 40in axial length, 33in diameter
- **Ten:** 10% average ^{235}U enrichment in cylindrical core

U233-SOL-THERM-008



- 48in diameter unreflected Aluminum sphere of ^{233}U Nitrate solution

SIZE

Reproduced from the ICSBEP Handbook (2015)

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MGMC can replicate deterministic multigroup criticality calculations to within statistical significance.

U233-SOL-THERM-008

P_N	k_{eff} PARTISN	k_{eff} DAT	$\Delta k_{\text{eff}}(\sigma)$	k_{eff} SC	$\Delta k_{\text{eff}}(\sigma)$
P_0	1.02819	1.02819± 5pcm	0.1	1.02819 ± 5pcm	0.1
P_1	0.99486	0.99493± 5pcm	1.2	0.99504 ± 5pcm	3.7
P_3	0.99503	0.99509± 5pcm	1.2	0.99504 ± 5pcm	0.1

- U233-SOL-THERM-008 simulations showed the best agreement between PARTISN and MGMC, likely due to large dimensions
  - discrepancies between PARTISN and MGMC decrease as truncation order increases for anisotropic scattering
  - we do not expect exact agreement between the two codes because higher order moments of low-order truncations are different

MGMC agrees well with PARTISN; anisotropic scattering agreement improves with increasing scattering order.

U233-SOL-THERM-008

P_N	k_{eff} PARTISN	k_{eff} DAT	$\Delta k_{\text{eff}}(\sigma)$	k_{eff} SC	$\Delta k_{\text{eff}}(\sigma)$
P_0	1.02819	1.02819± 5pcm	0.1	1.02819 ± 5pcm	0.1
P_1	0.99486	0.99493± 5pcm	1.2	0.99504 ± 5pcm	3.7
P_3	0.99503	0.99509± 5pcm	1.2	0.99504 ± 5pcm	0.1

IEU-MET-FAST-007

P_N	k_{eff} PARTISN	k_{eff} DAT	$\Delta k_{\text{eff}}(\sigma)$	k_{eff} SC	$\Delta k_{\text{eff}}(\sigma)$
P_0	1.04471	1.04466 ± 4pcm	1.3	1.04466 ± 4pcm	1.3
P_1	0.99283	0.99216 ± 4pcm	16.8	0.99312 ± 4pcm	7.7
P_3	0.99357	0.99348 ± 4pcm	2.1	0.99331 ± 4pcm	6.3

PU-MET-FAST-006

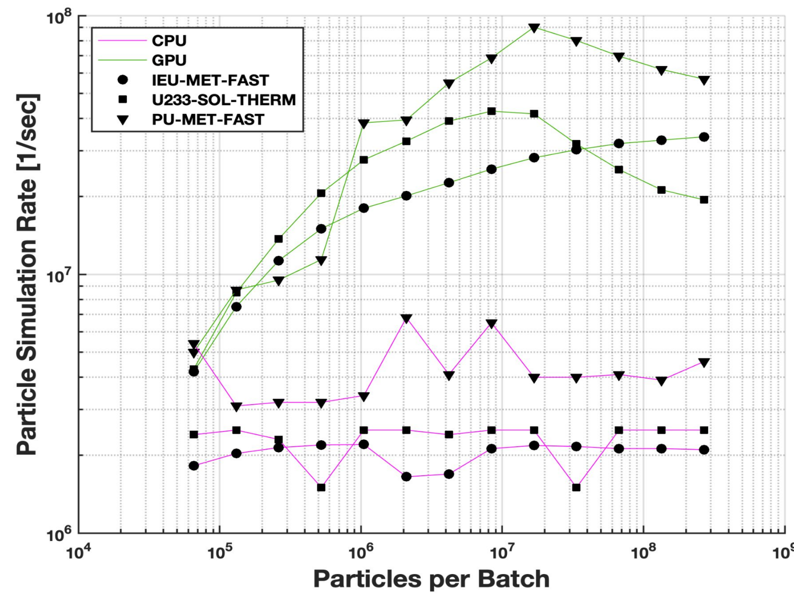
P_N	k_{eff} PARTISN	k_{eff} DAT	$\Delta k_{\text{eff}}(\sigma)$	k_{eff} SC	$\Delta k_{\text{eff}}(\sigma)$
P_0	1.14654	1.14652 ± 5pcm	0.3	1.14652 ± 5pcm	0.3
P_1	0.97238	0.96734 ± 4pcm	111.9	0.99157 ± 4pcm	436.0
P_3	0.99493	0.99468 ± 4pcm	5.8	0.99716 ± 5pcm	47.3

- PARTISN P_0 is a metric for the importance of scattering anisotropy
- We expect MGMC and PARTISN P_0 values to agree because they use the same scattering PDFs
- As the importance of anisotropy increases, PARTISN and MGMC show more disagreement for P_1 and P_3 simulations

Speedups of 15-25x have been demonstrated with the SC method on NVIDIA V100 GPUs.

- To assess performance, particle simulation rate can be used.
  - computed this rate for 2^{16} - 2^{29} neutrons per batch, 30 groups, P_3 SC sampling
  - tested on Sierra clone node
    - 2 Power9 CPUs, 4 NVIDIA V100 GPUs

- Additional simulations show that SC P_3 is only about 10% slower than P_0 sampling on GPUs, independent of number of groups used.



Parallelization on Sierra clone node
CPU: 4 MPI Processes, 40 OpenMP Threads/Proc
GPU: 4 MPI Processes, 1 NVIDIA Volta GPU/Proc

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Conclusions

- **Our problem**: Legendre truncations to multigroup scattering distributions are not amenable to Monte Carlo sampling due to negative values.

- **Our work**: We have implemented two moment-preserving methods in `MGMC` that
  - capture the shape of the truncation;
  - are non-negative over [-1, 1]; and
  - can be efficiently sampled on CPUs and GPUs

- **Our results**:
  - `MGMC` can now simulate neutrons with anisotropic scattering mechanics
  - `MGMC` shows good agreement with LANL production codes `PARTISN`

Future Work

- **Sampling methods**
  - Entropy-maximizing method
  - 5^{th} order semi-continuous PDFs

- **Future verification**
  - Verifying MGMC's results over more complex critical benchmarks
  - Comparing MGMC simulations with additional neutron transport codes

- **Performance**
  - Profiling MGMC's performance on GPUs
  - Testing performance on A100s
  - Experimenting with additional parallelization strategies

Thank you for listening!